

# Diffusion-based Molecule Generation with Informative Prior Bridges

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## Abstract

AI-based molecule generation provides a promising approach to a large area of biomedical sciences and engineering, such as antibody design, hydrolase engineering, or vaccine development. Because the molecules are governed by physical laws, a key challenge is to incorporate prior information into the training procedure to generate high-quality and realistic molecules. We propose a simple and novel approach to steer the training of diffusion-based generative models with physical and statistics prior information. This is achieved by constructing physically informed diffusion bridges, stochastic processes that guarantee to yield a given observation at the fixed terminal time. We develop a Lyapunov function based method to construct and determine bridges, and propose a number of proposals of informative prior bridges for both high-quality molecule generation and uniformity-promoted 3D point cloud generation. With comprehensive experiments, we show that our method provides a powerful approach to the 3D generation task, yielding molecule structures with better quality and stability scores and more uniformly distributed point clouds of high qualities.